



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2022 – 02:08 PM EDT

PDB ID : 6BSH
Title : Structure of HIV-1 RT complexed with RNA/DNA hybrid in the RNA hydrolysis mode
Authors : Tian, L.; Kim, M.; Yang, W.
Deposited on : 2017-12-03
Resolution : 2.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.27
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.27

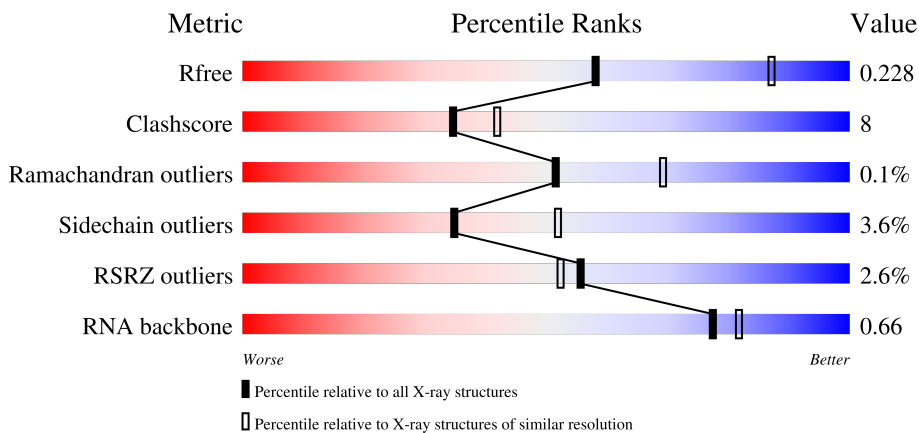
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)
RNA backbone	3102	1027 (2.96-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	558	 3% 78% 17% . .
2	B	441	 % 78% 13% . 8%
3	D	23	 9% 43% 57%
4	R	25	 4% 48% 36% 16%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	GOL	A	605	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8875 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called REVERSE TRANSCRIPTASE P66 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	544	4427	2862	738	819	8	0	4	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P03367
A	68	GLY	SER	conflict	UNP P03367
A	83	LYS	ARG	conflict	UNP P03367
A	357	MET	THR	conflict	UNP P03367
A	411	VAL	ILE	conflict	UNP P03367
A	461	LYS	ARG	conflict	UNP P03367
A	512	GLN	LYS	conflict	UNP P03367

- Molecule 2 is a protein called REVERSE TRANSCRIPTASE P51 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	404	3274	2130	532	606	6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A0A076Q3N8
B	68	GLY	SER	conflict	UNP A0A076Q3N8
B	83	LYS	ARG	conflict	UNP A0A076Q3N8
B	411	VAL	ILE	conflict	UNP A0A076Q3N8

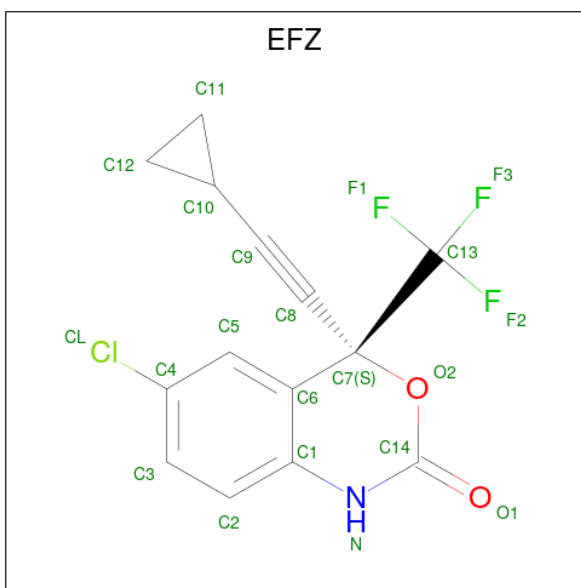
- Molecule 3 is a DNA chain called DNA (5'-D(*GP*TP*AP*TP*GP*CP*CP*AP*CP*TP*AP*GP*TP*TP*AP*TP*TP*GP*TP*GP*GP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	23	468	225	81	140	22	0	0	0

- Molecule 4 is a RNA chain called RNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	R	25	521	236	98	164	23	0	0	0

- Molecule 5 is (-)-6-CHLORO-4-CYCLOPROPYLETHYNYL-4-TRIFLUOROMETHYL-1,4-DIHYDRO-2H-3,1-BENZOXAZIN-2-ONE (three-letter code: EFZ) (formula: $C_{14}H_9ClF_3NO_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	F	N	O		
5	A	1	21	14	1	3	1	2	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

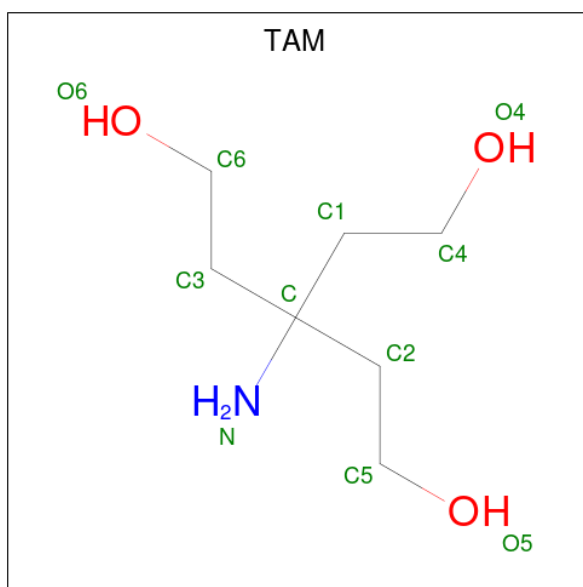
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	A	2	2	2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	R	1	11	7	1	3	0	0

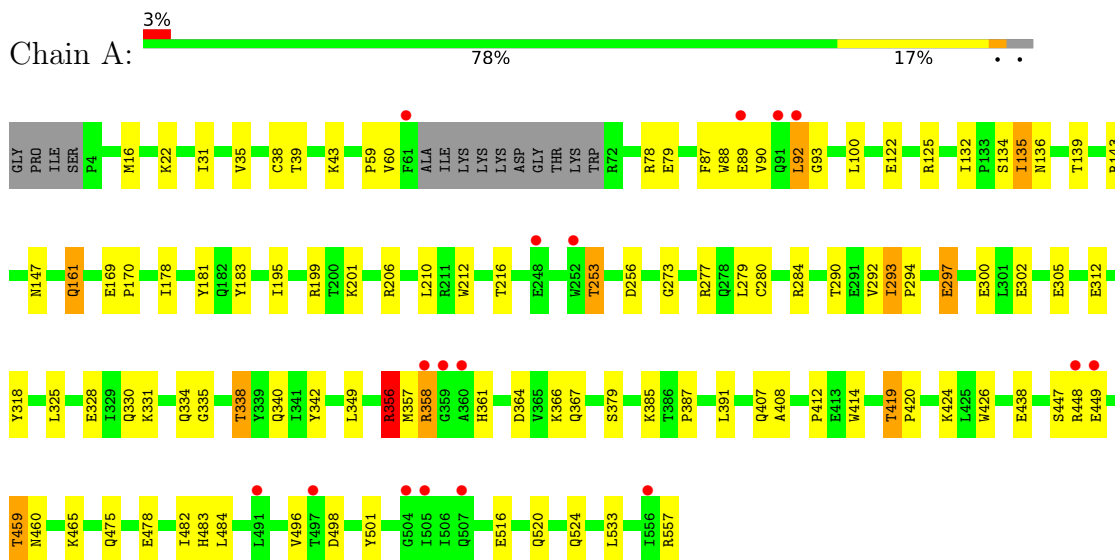
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	49	Total	O	0	0
			49	49		
9	B	40	Total	O	0	0
			40	40		
9	D	14	Total	O	0	0
			14	14		
9	R	12	Total	O	0	0
			12	12		

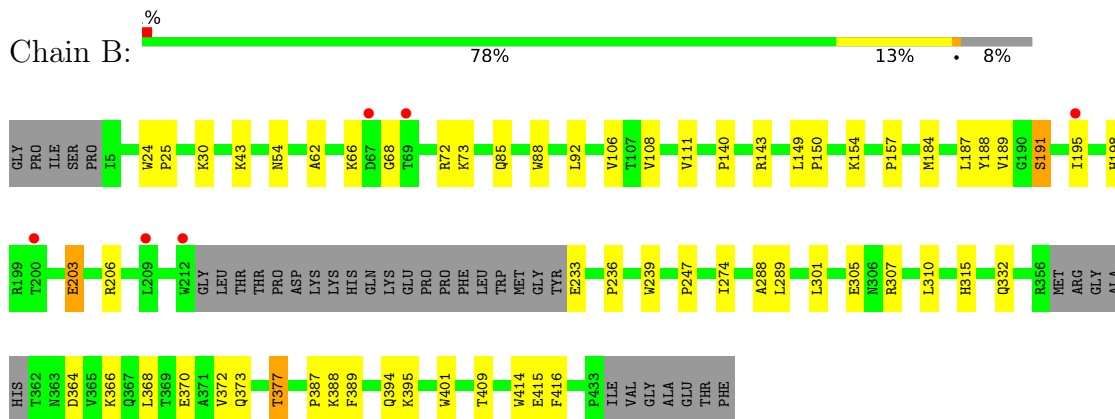
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

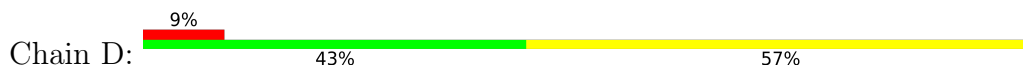
- Molecule 1: REVERSE TRANSCRIPTASE P66 SUBUNIT



- Molecule 2: REVERSE TRANSCRIPTASE P51 SUBUNIT

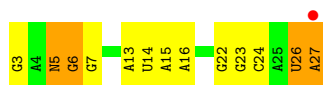


- Molecule 3: DNA (5'-D(*GP*TP*AP*TP*GP*CP*CP*AP*CP*TP*AP*GP*TP*TP*AP*TP*TP*GP*TP*GP*GP*CP*C)-3')





- Molecule 4: RNA (25-MER)



4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.79Å 161.79Å 128.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.20 – 2.65 37.20 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.20-2.65) 99.9 (37.20-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.65Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.189 , 0.227 0.190 , 0.228	Depositor DCC
R_{free} test set	2002 reflections (3.53%)	wwPDB-VP
Wilson B-factor (Å ²)	72.2	Xtrriage
Anisotropy	0.291	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8875	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: TAM, EFZ, 3DR, CA, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.56	2/4553 (0.0%)	0.62	2/6190 (0.0%)
2	B	0.46	1/3367 (0.0%)	0.56	0/4594
3	D	1.01	0/523	1.20	2/806 (0.2%)
4	R	0.62	0/570	1.20	3/883 (0.3%)
All	All	0.57	3/9013 (0.0%)	0.71	7/12473 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	356[A]	ARG	CA-C	14.82	1.91	1.52
1	A	356[B]	ARG	CA-C	14.82	1.91	1.52
2	B	203	GLU	CB-CG	8.11	1.67	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356[A]	ARG	CA-C-O	-7.51	104.33	120.10
1	A	356[B]	ARG	CA-C-O	-7.51	104.33	120.10
3	D	20	DG	O4'-C4'-C3'	-6.46	101.92	104.50
4	R	16	A	O5'-P-OP2	-6.04	100.26	105.70
4	R	15	A	OP2-P-O3'	5.89	118.17	105.20
4	R	14	U	OP2-P-O3'	5.42	117.12	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	10	DT	O4'-C4'-C3'	-5.23	102.41	104.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	356[A]	ARG	Mainchain
1	A	356[B]	ARG	Mainchain
1	A	88	TRP	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4427	0	4449	86	0
2	B	3274	0	3208	34	0
3	D	468	0	263	13	0
4	R	521	0	272	17	0
5	A	21	0	9	1	0
6	A	2	0	0	0	0
7	A	24	0	32	2	0
7	B	6	0	8	0	0
7	D	6	0	8	0	0
8	R	11	0	17	2	0
9	A	49	0	0	2	0
9	B	40	0	0	0	0
9	D	14	0	0	1	0
9	R	12	0	0	1	0
All	All	8875	0	8266	139	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (139) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:5:3DR:O4'	4:R:5:3DR:C4'	1.65	1.27
1:A:357:MET:O	1:A:358:ARG:HD2	1.41	1.20
1:A:356[B]:ARG:NH1	1:A:358:ARG:HA	1.56	1.18
1:A:356[B]:ARG:HH11	1:A:358:ARG:HA	1.14	0.91
3:D:4:DT:H2'	3:D:5:DG:C8	2.13	0.83
1:A:357:MET:O	1:A:358:ARG:CD	2.26	0.79
1:A:356[B]:ARG:NH1	1:A:358:ARG:CA	2.45	0.78
1:A:331:LYS:NZ	1:A:364:ASP:OD2	2.19	0.76
1:A:557:ARG:HG2	4:R:26:U:H5'	1.71	0.72
1:A:181[A]:TYR:CE2	1:A:183:TYR:HB2	2.25	0.71
1:A:325:LEU:HD12	1:A:385:LYS:HE2	1.72	0.70
3:D:12:DG:N3	9:D:201:HOH:O	2.24	0.70
4:R:6:G:H2'	4:R:7:G:H8	1.58	0.69
1:A:356[B]:ARG:HH12	1:A:358:ARG:HA	1.56	0.68
3:D:2:DT:H3	4:R:27:A:H62	1.42	0.67
1:A:356[B]:ARG:HH11	1:A:358:ARG:CA	2.00	0.64
7:A:607:GOL:O3	7:A:607:GOL:O1	2.01	0.64
1:A:284:ARG:NH1	9:A:703:HOH:O	2.29	0.63
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.63	0.62
3:D:4:DT:H2'	3:D:5:DG:H8	1.63	0.61
1:A:92:LEU:H	1:A:92:LEU:HD23	1.65	0.61
2:B:373:GLN:O	2:B:377:THR:HG23	2.01	0.61
1:A:357:MET:N	1:A:357:MET:SD	2.76	0.59
3:D:6:DC:H41	8:R:101:TAM:H12	1.66	0.59
4:R:5:3DR:H2'	9:R:212:HOH:O	2.01	0.59
4:R:6:G:H2'	4:R:7:G:C8	2.38	0.59
1:A:424:LYS:HE3	1:A:426:TRP:CZ3	2.38	0.59
4:R:6:G:OP1	4:R:6:G:H8	1.86	0.58
1:A:293:ILE:HD12	1:A:294:PRO:HD2	1.85	0.57
1:A:357:MET:C	1:A:358:ARG:HD2	2.23	0.56
1:A:277[B]:ARG:HH22	1:A:356[B]:ARG:HH22	1.53	0.56
1:A:181[A]:TYR:CD2	5:A:601:EFZ:H101	2.42	0.55
2:B:366:LYS:O	2:B:370:GLU:HG3	2.08	0.54
3:D:1:DG:H2'	3:D:1:DG:N3	2.21	0.54
1:A:356[A]:ARG:HG2	1:A:358:ARG:H	1.73	0.54
1:A:438:GLU:OE1	1:A:459:THR:HG21	2.07	0.53
1:A:273:GLY:HA2	1:A:338:THR:HG21	1.88	0.53
3:D:1:DG:H2''	3:D:2:DT:C4	2.44	0.52
1:A:100:LEU:O	1:A:318:TYR:HB3	2.10	0.52
2:B:388:LYS:HZ1	2:B:415:GLU:CD	2.13	0.52
3:D:6:DC:N4	8:R:101:TAM:H12	2.24	0.52
1:A:253:THR:HG22	1:A:256:ASP:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:SER:OG	1:A:387:PRO:HD3	2.09	0.52
1:A:280:CYS:SG	4:R:13:A:H4'	2.50	0.51
1:A:39:THR:O	1:A:43:LYS:HE2	2.10	0.50
1:A:357:MET:O	1:A:358:ARG:CB	2.59	0.50
1:A:279:LEU:HD12	1:A:302:GLU:OE1	2.11	0.50
1:A:460:ASN:HD22	2:B:288:ALA:HB2	1.77	0.49
1:A:460:ASN:ND2	2:B:288:ALA:HB2	2.27	0.49
1:A:335:GLY:HA3	1:A:356[B]:ARG:HG2	1.94	0.49
2:B:203:GLU:O	2:B:206:ARG:N	2.46	0.49
4:R:5:3DR:O4'	4:R:5:3DR:C5'	2.53	0.49
4:R:6:G:H8	4:R:6:G:P	2.36	0.49
2:B:108:VAL:HG22	2:B:188:TYR:CD2	2.48	0.48
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.94	0.48
1:A:195:ILE:O	1:A:199:ARG:HG3	2.13	0.48
2:B:301:LEU:O	2:B:305:GLU:HG3	2.14	0.47
1:A:478:GLU:O	1:A:482:ILE:HG13	2.13	0.47
2:B:72:ARG:HG2	2:B:73:LYS:N	2.30	0.47
1:A:277[B]:ARG:NH1	1:A:334:GLN:O	2.46	0.46
2:B:43:LYS:HE3	2:B:43:LYS:HB2	1.74	0.46
1:A:498:ASP:O	4:R:24:C:H5'	2.15	0.46
1:A:412:PRO:HG2	2:B:401:TRP:CH2	2.50	0.46
1:A:448:ARG:HG3	1:A:448:ARG:HH11	1.80	0.46
3:D:1:DG:H2''	3:D:2:DT:C5	2.51	0.46
1:A:206:ARG:HD2	1:A:216:THR:OG1	2.16	0.46
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.50	0.46
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.56	0.46
1:A:483:HIS:ND1	1:A:524:GLN:OE1	2.46	0.46
4:R:23:G:H2'	4:R:24:C:O4'	2.15	0.46
1:A:90:VAL:HG21	1:A:161:GLN:CD	2.37	0.46
2:B:191:SER:HB3	2:B:198:HIS:CE1	2.50	0.46
2:B:88:TRP:CH2	2:B:154:LYS:HD3	2.51	0.45
1:A:169:GLU:HB2	1:A:170:PRO:HD3	1.97	0.45
1:A:143:ARG:HG2	1:A:143:ARG:NH1	2.32	0.45
1:A:297:GLU:HA	1:A:300:GLU:HB2	1.98	0.45
1:A:90:VAL:HG21	1:A:161:GLN:OE1	2.17	0.45
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.17	0.45
2:B:233:GLU:N	2:B:233:GLU:OE2	2.50	0.45
1:A:449:GLU:H	1:A:449:GLU:CD	2.21	0.44
4:R:22:G:H2'	4:R:23:G:C8	2.52	0.44
1:A:178:ILE:HD11	1:A:201:LYS:HG3	1.99	0.44
1:A:356[A]:ARG:HH21	1:A:367:GLN:HE22	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLU:HG2	1:A:330:GLN:OE1	2.17	0.44
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.32	0.44
1:A:122:GLU:O	1:A:125:ARG:HG3	2.18	0.44
1:A:125:ARG:HD3	1:A:147:ASN:HA	2.00	0.43
1:A:253:THR:HG22	1:A:256:ASP:CG	2.38	0.43
4:R:6:G:OP1	4:R:6:G:C8	2.69	0.43
2:B:88:TRP:CZ2	2:B:154:LYS:HD3	2.54	0.43
1:A:181[A]:TYR:HE2	1:A:183:TYR:HB2	1.81	0.43
2:B:106:VAL:HA	2:B:189:VAL:O	2.19	0.43
1:A:253:THR:CG2	1:A:256:ASP:H	2.31	0.43
2:B:368:LEU:O	2:B:372:VAL:HG23	2.19	0.43
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.80	0.43
1:A:366:LYS:HE3	1:A:407:GLN:OE1	2.18	0.43
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.54	0.43
3:D:2:DT:H1'	3:D:3:DA:H5'	2.01	0.43
1:A:135:ILE:HD12	1:A:136:ASN:H	1.83	0.43
1:A:408:ALA:HB1	2:B:364:ASP:HB3	2.00	0.43
2:B:111:VAL:O	2:B:111:VAL:HG12	2.19	0.43
1:A:357:MET:O	1:A:358:ARG:HB2	2.18	0.42
4:R:6:G:C2	4:R:7:G:C4	3.07	0.42
1:A:92:LEU:HG	1:A:93:GLY:H	1.85	0.42
1:A:424:LYS:HE3	1:A:426:TRP:HZ3	1.82	0.42
2:B:30:LYS:HE2	2:B:62:ALA:O	2.20	0.42
1:A:22:LYS:HB2	1:A:22:LYS:HE3	1.84	0.42
1:A:419:THR:O	1:A:419:THR:OG1	2.37	0.42
1:A:419:THR:HA	1:A:420:PRO:HD2	1.94	0.42
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.93	0.42
2:B:24:TRP:CG	2:B:25:PRO:HD2	2.55	0.41
1:A:59:PRO:HB3	4:R:3:G:C6	2.54	0.41
1:A:212:TRP:NE1	7:A:605:GOL:H11	2.36	0.41
1:A:516:GLU:O	1:A:520:GLN:HG3	2.20	0.41
1:A:340:GLN:HG2	9:A:714:HOH:O	2.19	0.41
1:A:465:LYS:HE3	1:A:484:LEU:HD13	2.02	0.41
1:A:496:VAL:HG21	2:B:289:LEU:HD21	2.03	0.41
1:A:161:GLN:HE22	2:B:140:PRO:HG3	1.85	0.41
2:B:54:ASN:O	2:B:143:ARG:NH2	2.53	0.41
3:D:8:DA:H2'	3:D:9:DC:C6	2.55	0.41
1:A:273:GLY:CA	1:A:338:THR:HG21	2.51	0.41
1:A:330:GLN:HE22	1:A:340:GLN:HE22	1.68	0.41
3:D:14:DT:H2''	3:D:15:DA:O5'	2.21	0.41
2:B:157:PRO:HG3	2:B:184:MET:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:O	1:A:35:VAL:HG13	2.21	0.41
2:B:274:ILE:HD11	2:B:310:LEU:HD21	2.02	0.41
3:D:1:DG:O6	4:R:27:A:H2'	2.20	0.41
1:A:391:LEU:HD12	1:A:414:TRP:CE3	2.56	0.41
2:B:247:PRO:O	2:B:307:ARG:NH2	2.53	0.41
1:A:87:PHE:HB2	1:A:89:GLU:HG3	2.03	0.40
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.56	0.40
1:A:305:GLU:H	1:A:305:GLU:HG3	1.70	0.40
1:A:134:SER:OG	1:A:139:THR:HB	2.20	0.40
2:B:66:LYS:C	2:B:68:GLY:H	2.25	0.40
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	544/558 (98%)	523 (96%)	20 (4%)	1 (0%)	47	64
2	B	398/441 (90%)	388 (98%)	10 (2%)	0	100	100
All	All	942/999 (94%)	911 (97%)	30 (3%)	1 (0%)	51	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	ARG

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	483/496 (97%)	461 (95%)	22 (5%)	27	41
2	B	352/399 (88%)	343 (97%)	9 (3%)	46	65
All	All	835/895 (93%)	804 (96%)	31 (4%)	35	51

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	MET
1	A	60	VAL
1	A	78	ARG
1	A	79	GLU
1	A	92	LEU
1	A	135	ILE
1	A	161	GLN
1	A	210	LEU
1	A	253	THR
1	A	290	THR
1	A	292	VAL
1	A	293	ILE
1	A	297	GLU
1	A	312	GLU
1	A	338	THR
1	A	356[A]	ARG
1	A	356[B]	ARG
1	A	361	HIS
1	A	419	THR
1	A	447	SER
1	A	459	THR
1	A	533	LEU
2	B	92	LEU
2	B	191	SER
2	B	195	ILE
2	B	315	HIS
2	B	332	GLN
2	B	377	THR
2	B	394	GLN
2	B	409	THR
2	B	414	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	R	22/25 (88%)	3 (13%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	R	6	G
4	R	26	U
4	R	27	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	3DR	R	5	4	8,11,12	5.69	6 (75%)	9,14,17	1.77	2 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	3DR	R	5	4	-	2/3/15/16	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	5	3DR	O4'-C4'	12.96	1.65	1.44
4	R	5	3DR	C3'-C4'	-7.40	1.32	1.53
4	R	5	3DR	O4'-C1'	-4.37	1.29	1.42
4	R	5	3DR	C2'-C1'	2.52	1.58	1.51
4	R	5	3DR	O5'-C5'	-2.35	1.39	1.44
4	R	5	3DR	O3'-C3'	2.05	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	5	3DR	C1'-C2'-C3'	-3.96	98.73	103.20
4	R	5	3DR	O4'-C1'-C2'	-2.19	101.94	106.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	R	5	3DR	C3'-C4'-C5'-O5'
4	R	5	3DR	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	5	3DR	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
7	GOL	A	607	-	5,5,5	0.31	0	5,5,5	0.58	0
7	GOL	D	101	-	5,5,5	0.42	0	5,5,5	0.53	0
5	EFZ	A	601	-	23,23,23	5.79	9 (39%)	36,36,36	5.18	22 (61%)
7	GOL	B	501	-	5,5,5	0.28	0	5,5,5	0.42	0
7	GOL	A	604	-	5,5,5	0.42	0	5,5,5	0.22	0
8	TAM	R	101	-	7,10,10	1.16	0	9,12,12	1.10	1 (11%)
7	GOL	A	605	-	5,5,5	0.43	0	5,5,5	0.78	0
7	GOL	A	606	-	5,5,5	0.30	0	5,5,5	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. ^{1,2} means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	607	-	-	1/4/4/4	-
7	GOL	D	101	-	-	2/4/4/4	-
5	EFZ	A	601	-	-	0/10/32/32	0/3/3/3
7	GOL	B	501	-	-	1/4/4/4	-
7	GOL	A	604	-	-	2/4/4/4	-
8	TAM	R	101	-	-	1/12/12/12	-
7	GOL	A	605	-	-	2/4/4/4	-
7	GOL	A	606	-	-	0/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	EFZ	C1-C6	18.71	1.61	1.40
5	A	601	EFZ	C12-C11	11.12	1.90	1.48
5	A	601	EFZ	C7-C6	8.01	1.61	1.51
5	A	601	EFZ	C5-C4	-7.74	1.25	1.38
5	A	601	EFZ	C3-C4	-7.28	1.24	1.38
5	A	601	EFZ	C2-C1	7.28	1.52	1.39
5	A	601	EFZ	C10-C9	5.64	1.65	1.46
5	A	601	EFZ	O2-C7	-3.69	1.39	1.45
5	A	601	EFZ	C7-C8	2.42	1.54	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	EFZ	C2-C1-C6	-17.34	102.83	119.88
5	A	601	EFZ	C2-C1-N	11.82	140.05	119.84
5	A	601	EFZ	C12-C10-C11	10.76	89.74	59.23
5	A	601	EFZ	O2-C7-C6	-9.18	105.16	111.64
5	A	601	EFZ	C7-O2-C14	7.52	135.11	121.44
5	A	601	EFZ	C11-C12-C10	-6.25	45.00	60.38
5	A	601	EFZ	C12-C11-C10	-6.14	45.26	60.38
5	A	601	EFZ	C3-C4-CL	-4.82	111.81	119.35
5	A	601	EFZ	O2-C14-O1	4.75	125.21	118.02
5	A	601	EFZ	O2-C7-C13	4.45	112.97	104.76
5	A	601	EFZ	C5-C6-C1	4.24	124.06	118.72
5	A	601	EFZ	F1-C13-C7	-4.19	106.66	111.79
5	A	601	EFZ	C2-C3-C4	3.82	123.27	119.24
5	A	601	EFZ	C12-C10-C9	-3.28	110.14	119.06
5	A	601	EFZ	C3-C4-C5	3.24	125.84	121.53
5	A	601	EFZ	C5-C6-C7	-2.68	119.60	122.71
5	A	601	EFZ	F3-C13-C7	-2.59	108.63	111.79
5	A	601	EFZ	C5-C4-CL	2.56	122.35	119.15
5	A	601	EFZ	C13-C7-C8	-2.53	104.82	108.89
5	A	601	EFZ	F2-C13-C7	2.39	114.72	111.79
8	R	101	TAM	C2-C-C1	-2.30	106.45	110.50
5	A	601	EFZ	C6-C1-N	-2.19	117.12	119.88
5	A	601	EFZ	C3-C2-C1	2.09	123.68	119.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

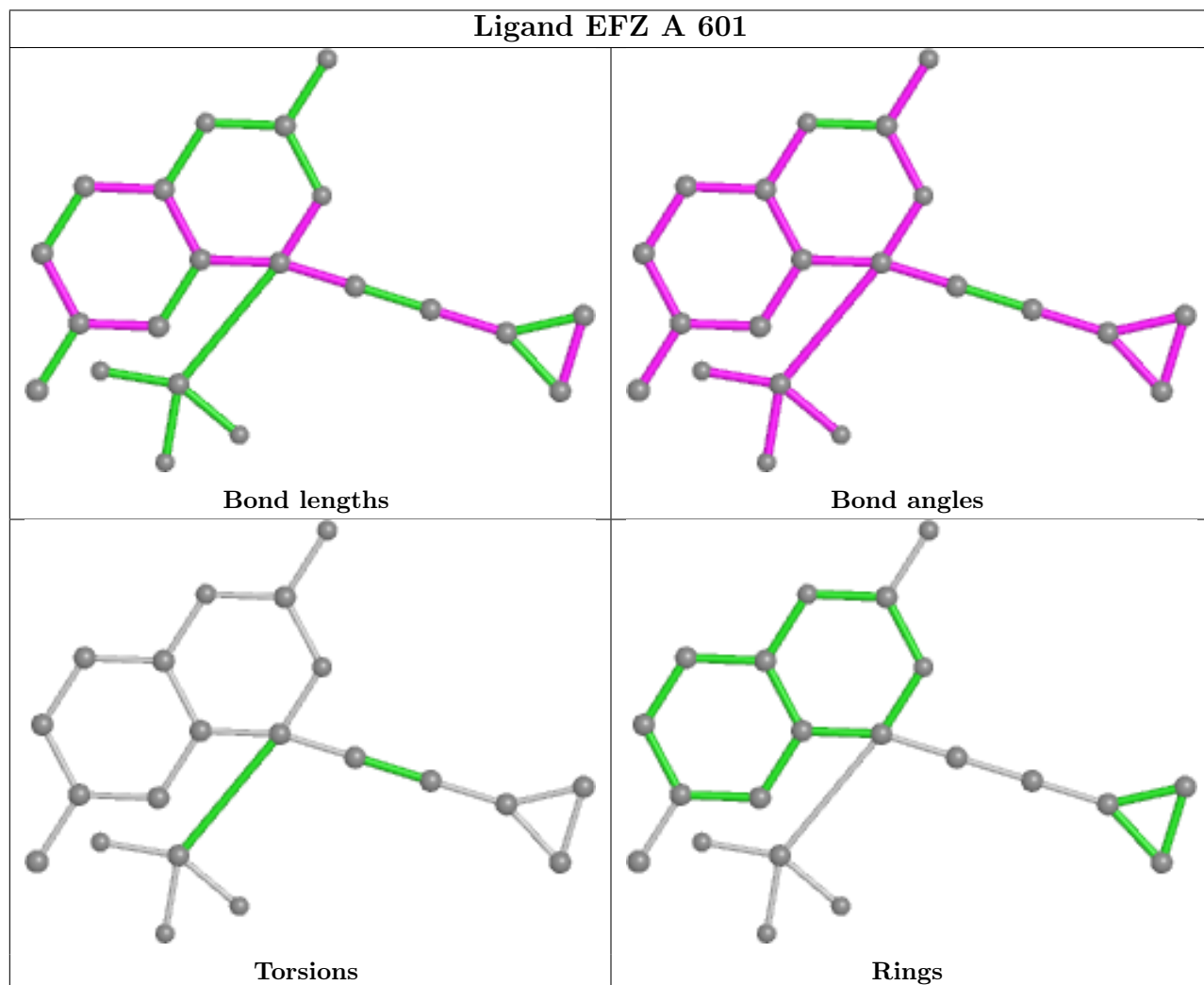
Mol	Chain	Res	Type	Atoms
7	A	604	GOL	O1-C1-C2-C3
7	A	605	GOL	O1-C1-C2-C3
7	D	101	GOL	O1-C1-C2-C3
8	R	101	TAM	C-C2-C5-O5
7	A	607	GOL	O1-C1-C2-C3
7	B	501	GOL	O1-C1-C2-C3
7	A	604	GOL	O1-C1-C2-O2
7	A	605	GOL	O1-C1-C2-O2
7	D	101	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	607	GOL	1	0
5	A	601	EFZ	1	0
8	R	101	TAM	2	0
7	A	605	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	544/558 (97%)	-0.04	17 (3%) 49 45	47, 67, 103, 133	0
2	B	404/441 (91%)	-0.12	6 (1%) 73 71	48, 74, 135, 152	0
3	D	23/23 (100%)	-0.18	2 (8%) 10 8	49, 63, 110, 137	0
4	R	24/25 (96%)	-0.68	1 (4%) 36 33	56, 62, 107, 128	0
All	All	995/1047 (95%)	-0.09	26 (2%) 56 52	47, 70, 118, 152	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	359	GLY	4.3
2	B	69	THR	4.2
2	B	212	TRP	3.7
3	D	1	DG	3.6
2	B	67	ASP	3.6
2	B	200	THR	3.5
3	D	2	DT	3.4
1	A	448	ARG	3.1
1	A	252	TRP	3.0
1	A	89	GLU	3.0
1	A	91	GLN	2.7
1	A	449	GLU	2.7
1	A	360	ALA	2.7
1	A	491	LEU	2.6
1	A	556	ILE	2.6
2	B	209	LEU	2.6
4	R	27	A	2.4
1	A	358	ARG	2.3
1	A	248	GLU	2.2
1	A	92	LEU	2.2
1	A	497	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	505	ILE	2.1
2	B	195	ILE	2.1
1	A	61	PHE	2.1
1	A	507	GLN	2.1
1	A	504	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	3DR	R	5	11/12	0.92	0.17	84,113,125,137	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

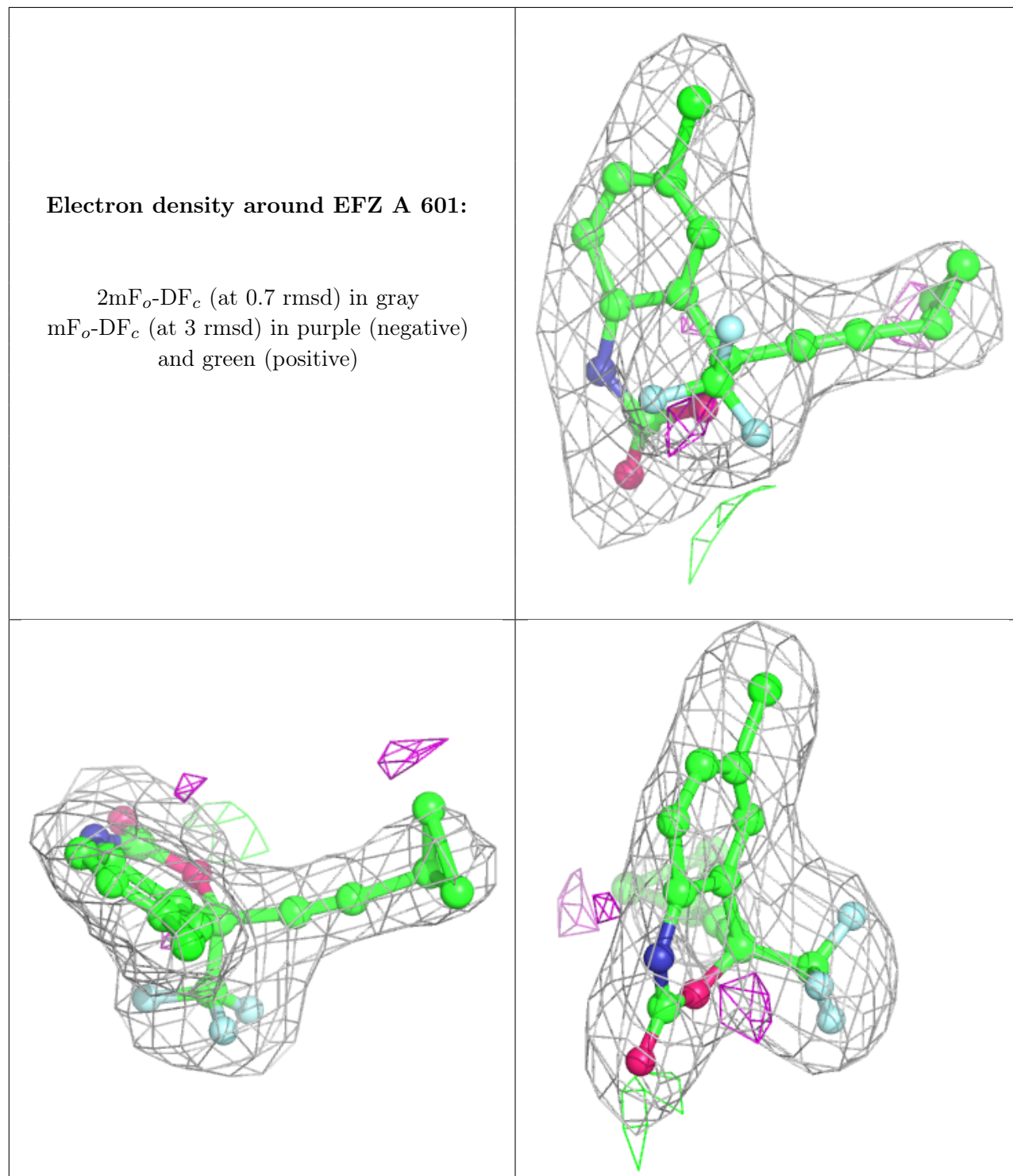
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	A	606	6/6	0.71	0.31	88,95,102,103	0
7	GOL	A	605	6/6	0.72	0.42	77,81,85,89	0
8	TAM	R	101	11/11	0.80	0.33	69,76,84,88	0
7	GOL	D	101	6/6	0.84	0.33	75,86,88,89	0
7	GOL	B	501	6/6	0.87	0.18	66,74,81,82	0
7	GOL	A	604	6/6	0.88	0.13	73,79,87,91	0
7	GOL	A	607	6/6	0.90	0.27	69,75,88,96	0
5	EFZ	A	601	21/21	0.97	0.16	44,56,65,68	0
6	CA	A	602	1/1	0.98	0.10	69,69,69,69	0
6	CA	A	603	1/1	0.99	0.17	63,63,63,63	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.